

Succinic acid, 2,2-dimethylpent-3-yl isobutyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C15H28O4/c1-7-12(15(4,5)6)19-14(17)9-8-13(16)18-10-11(2)3/h11-12H,7-10H |
| InchiKey: | JEASZTJVUXRRHU-UHFFFAOYSA-N |
| Formula: | C15H28O4 |
| SMILES: | CCC(OC(=O)CCC(=O)OCC(C)C)C(C)(C)C |
| Mol. weight [g/mol]: | 272.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -394.46 | kJ/mol | Joback Method |
| hf | -861.84 | kJ/mol | Joback Method |
| hfus | 25.72 | kJ/mol | Joback Method |
| hvap | 65.22 | kJ/mol | Joback Method |
| log10ws | -3.45 | | Crippen Method |
| logp | 3.334 | | Crippen Method |
| mcvol | 237.090 | ml/mol | McGowan Method |
| pc | 1561.05 | kPa | Joback Method |
| rinpol | 1647.00 | | NIST Webbook |
| rinpol | 1647.00 | | NIST Webbook |
| tb | 691.07 | K | Joback Method |
| tc | 878.32 | K | Joback Method |
| tf | 375.55 | K | Joback Method |
| vc | 0.900 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 680.58 | J/molxK | 691.07 | Joback Method |
| cpg | 756.61 | J/molxK | 847.11 | Joback Method |
| cpg | 743.16 | J/molxK | 815.90 | Joback Method |
| cpg | 728.85 | J/molxK | 784.70 | Joback Method |
| cpg | 713.66 | J/molxK | 753.49 | Joback Method |
| cpg | 697.58 | J/molxK | 722.28 | Joback Method |
| cpg | 769.22 | J/molxK | 878.32 | Joback Method |
| dvisc | 0.0000764 | Paxs | 691.07 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001064 | Paxs | 638.48 | Joback Method |
| dvisc | 0.0001571 | Paxs | 585.90 | Joback Method |
| dvisc | 0.0002507 | Paxs | 533.31 | Joback Method |
| dvisc | 0.0004430 | Paxs | 480.72 | Joback Method |
| dvisc | 0.0009002 | Paxs | 428.14 | Joback Method |
| dvisc | 0.0022315 | Paxs | 375.55 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381730&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/90-090-2/Succinic-acid-2-2-dimethylpent-3-yl-isobutyl-ester.pdf>

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